Validation of SNPP NUCAPS trace gas EDRs: O_3, CO, and CO_2

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  - **NOAA AEROSE:** E. Joseph, V. R. Morris, M. Oyola (HU/NCAS); D. Wolfe (NOAA/ESRL)
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  - **World Ozone and Ultraviolet Radiation Data Centre (WOUDC)** data contributors (DWD-GRUAN, & INPE, & KNMI, & NASA-WFF, & SMNA. http://www.woudc.org
  - **SHADOZ: Southern Hemisphere ADditional Ozonesondes** (A. Thompson et al.)

- **NUCAPS validation effort (past and present)**: M. Wilson, T. King, W. W. Wolf, A.K. Sharma (STAR)

Outline

- **JPSS Sounder Trace Gas EDR Cal/Val Overview**
  - JPSS Level 1 Requirements
  - Validation Hierarchy
  - NUCAPS Algorithm
    - v1.5 (operational, CrIS nominal res)
    - v1.8.1. (CrIS full-res)
- **NUCAPS IR Ozone Profile EDR Product Evaluation**
  - v1.5 (operational)
    - Global Focus Day
    - Ozonesonde ensemble
  - v1.8.1 (CrIS full-res)
    - Global Focus Day
- **NUCAPS Trace Gas EDR Product Evaluation Versus AIRS v6 (Preliminary)**
  - Basic Methodology
  - Carbon Monoxide (CO)
    - v1.5 (operational)
    - v1.8.1 (full-res CrIS)
  - Carbon Dioxide (CO_2)
    - v1.5 (operational)
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- **Summary and Future Work**

JPSS Specification Performance Requirements
CrIS Trace Gas EDR Uncertainty (O_3, CO, CO_2, CH_4)

CrIS Infrared Trace Gases Specification Performance Requirements		
PARAMETER	**THRESHOLD**	**OBJECTIVE**
O_3 (Ozone) Profile Precision, 4–260 hPa (6 statistic layers)	20%	10%
O_3 (Ozone) Profile Precision, 260 hPa to sfc (1 statistic layer)	20%	10%
O_3 (Ozone) Profile Accuracy, 4–260 hPa (6 statistic layers)	±10%	±5%
O_3 (Ozone) Profile Accuracy, 260 hPa to sfc (1 statistic layer)	±10%	±5%
O_3 (Ozone) Profile Uncertainty, 4–260 hPa (6 statistic layers)	25%	15%
O_3 (Ozone) Profile Uncertainty, 260 hPa to sfc (1 statistic layer)	25%	15%
CO (Carbon Monoxide) Total Column Precision	35%, or full res mode 15%	3%
CO (Carbon Monoxide) Total Column Accuracy	±25%, or full res mode ±5%	±5%
CO_2 (Carbon Dioxide) Total Column Precision	0.5% (2 ppmv)	1.05 to 1.4 ppmv
CO_2 (Carbon Dioxide) Total Column Accuracy	±1% (4 ppmv)	NS
CH_4 (Methane) Total Column Precision	1% (≈20 ppbv)	NS
CH_4 (Methane) Total Column Accuracy	±4% (≈80 ppmv)	NS

Source:
(L1RD, 2014, pp. 45-49)

Validation Methodology Hierarchy

(e.g., *Nalli et al., JGR Special Section,* 2013)

1. **Numerical Model (e.g., ECMWF, NCEP/GFS) Global *Comparisons***
   - Large, truly global samples acquired from Focus Days
   - Useful for sanity checks, bias tuning and regression
   - Limitation: *Not* independent truth data

2. **Satellite Sounder EDR (e.g., AIRS, ATOVS, COSMIC) *Intercomparisons***
   - Global samples acquired from Focus Days (e.g., AIRS)
   - Consistency checks; merits of different retrieval algorithms
   - Limitation: Similar error characteristics; must take rigorous account of averaging kernels of both systems (e.g., *Rodgers and Connor,* 2003)

3. **Conventional RAOB Matchup *Assessments***
   - WMO/GTS operational sondes launched ~2/day for NWP
   - Representation of global zones, long-term monitoring
   - Large samples after a couple months (e.g., *Divakarla et al.,* 2006; *Reale et al.* 2012)
   - Limitations:
     - Skewed distribution toward NH-continents
     - Mismatch errors, potentially systematic at individual sites
     - Non-uniform, less-accurate and poorly characterized radiosondes
     - RAOBs assimilated , by definition, into numerical models

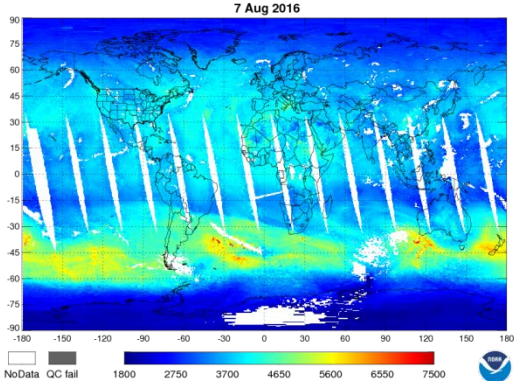
4. **Dedicated/Reference RAOB Matchup *Assessments***
   - *Dedicated* for the purpose of satellite validation
     - Known measurement uncertainty and optimal accuracy
     - Minimal mismatch errors
     - Atmospheric state “best estimates” or “merged soundings”
   - Reference sondes: CFH, **GRUAN** corrected RS92/RS41
     - Traceable measurement
     - Uncertainty estimates
   - Limitation: Small sample sizes and limited geographic coverage
   - E.g., **ARM sites** (e.g., *Tobin et al.,* 2006), **AEROSE**, **CalWater/ACAPEX ,** BCCSO, PMRF

5. **Intensive Field Campaign *Dissections***
   - Include dedicated RAOBs, some *not* assimilated into NWP models
   - Include ancillary datasets (e.g., ozonesondes, lidar, M-AERI, MWR, sunphotometer, etc.)
   - Ideally include funded aircraft campaign using IR sounder (e.g., NAST-I, S-HIS)
   - Detailed performance specification; state specification; SDR cal/val; case studies
   - E.g., **SNAP, SNPP-1,-2, AEROSE, CalWater/ACAPEX**, JAIVEX, WAVES, AWEX-G, EAQUATE

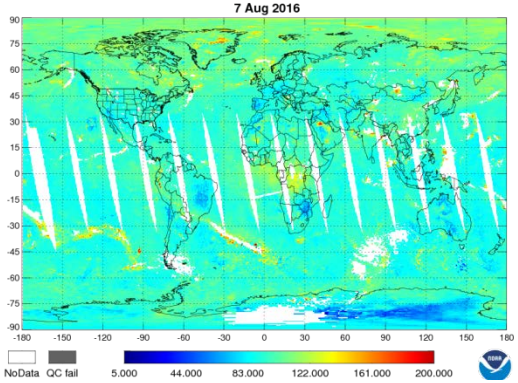
NOAA Unique Combined Atmospheric Processing System (NUCAPS) Algorithm (1/2)

- **Operational algorithm**
  - Unified Sounder Science Team (AIRS/IASI/CrIS) retrieval algorithm (*Susskind, Barnet and Blaisdell,* IEEE 2003; *Gambacorta et al.,* 2014)
  - Global non-precipitating conditions
  - Atmospheric Vertical Temperature , Moisture Profiles (**AVTP**, **AVMP**) and **trace gas** (**O_3, CO, CO_2, CH_4**)
  - Validated Maturity for AVTP/AVMP, Sep 2014
- **Users**
  - **Weather Forecast Offices (AWIPS)**
    - Nowcasting / severe weather
    - Alaska (cold core)
  - NOAA/CPC (OLR)
  - NOAA/ARL (IR ozone, trace gases)
  - TOAST (IR ozone)
  - Basic and applied science research (e.g., *Pagano et al.,* 2014)
    - Via NOAA Data Centers (e.g., CLASS)
    - Universities, peer-reviewed pubs

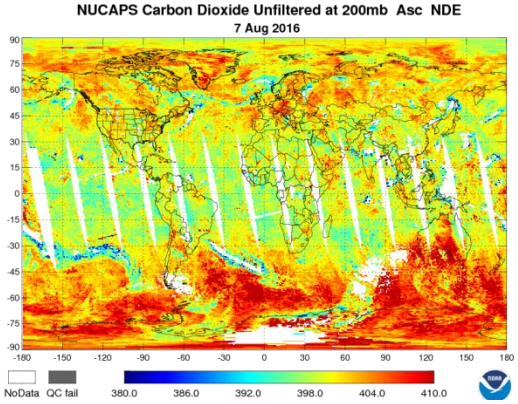
NUCAPS IR O_3



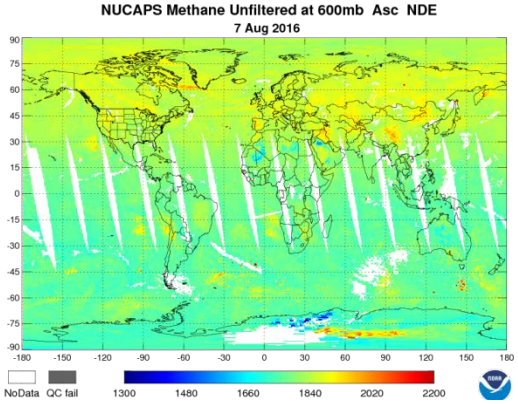
NUCAPS CO



NUCAPS CO_2



NUCAPS CH_4



Long Term Monitoring

http://www.star.nesdis.noaa.gov/jpss/EDRs/products_Soundings.php

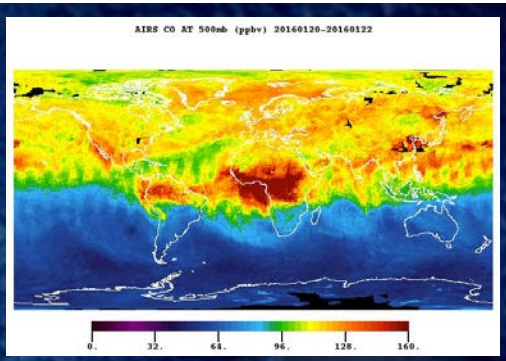
http://www.ospo.noaa.gov/Products/atmosphere/soundings/nucaps/index.html

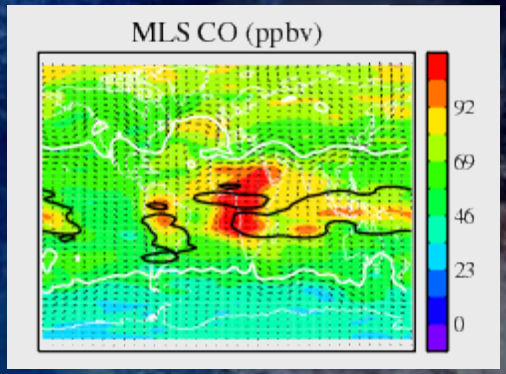
NOAA Unique Combined Atmospheric Processing System (NUCAPS) Algorithm (2/2)

- **NUCAPS Offline Code Versioning**
  - **Version 1.5**
    - **Current operational system**
    - Runs on **nominal CrIS spectral resolution** data
  - **Version 1.8.1**
    - **Offline experimental** algorithm
    - Runs on **CrIS full spectral resolution** data
    - Uses conventional regression algorithm for the IR/MW first guess (as opposed to MW retrieval as in v1.7 full-res)
    - Upgrades
      - Updated IR radiative transfer algorithm (RTA) bias correction coefficients (based on the best combination resulted after testing the use of several atmospheric states and trace gaseous profiles)
      - IR emissivity threshold decreased from 1.05 to 1.0 in the `temp_cris.nl` namelist.
      - Replaced the Taylor expansion to the Exponential formula in the `fasttau_co2.F` program.
      - Updated MW bias correction (as in v1.6)
      - Updated MW RTA model error coefficients (as in v1.6)
      - Removal of MW channel 16 (as in v1.6)

Validation of Products
NUCAPS EDR: Trace Gases (1/2)

- **Satellite Intercomparisons** (Hierarchy Method #2)
  - » **Aqua AIRS** (NASA A-Train)
    - Launched in 2002, the satellite sounder community has the experience of 13+ years of AIRS processing and AIRS has been well tested and validated
    - The Aqua satellite is in the same orbit as SNPP, thereby facilitating collocations with SNPP CrIS/ATMS
    - AIRS produces the same trace gas products as NUCAPS: **O_3, CO, CO_2, CH_4**
  - » **Orbiting Carbon Observatory (OCO)-2** (NASA A-Train)
    - Launched in July 2014
    - Provides **CO_2 observations**
  - » **Microwave Limb Sounder (MLS)** (NASA A-Train)
    - Launched in July 2004
    - Provides **CO observations**





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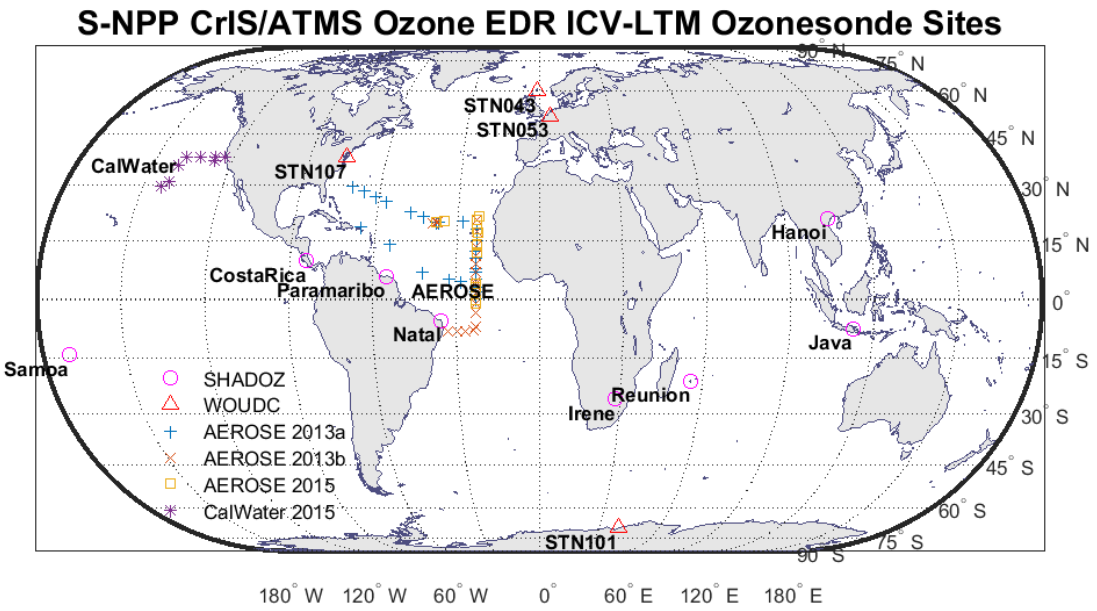
Validation of SNPP NUCAPS trace gas EDRs

IR OZONE PROFILE EDR

IR Ozone Profile EDR Validation (1/8)

In Situ Truth Datasets

- **Collocated ozonesondes** for **O_3 (ozone) profile EDR**
  - **Dedicated Ozonesondes**
    - **NOAA AEROSE** (*Nalli et al.* 2011)
    - **CalWater/ACAPEX 2015**
  - **Sites of Opportunity**
    - **SHADOZ** (*Thompson et al.* 2007)
      - Costa Rica
      - Hanoi
      - Irene
      - Java
      - Natal
      - Paramaribo
      - Reunion
      - American Samoa
    - **WOUDC**
      - STN043
      - STN053
      - STN107
      - STN101



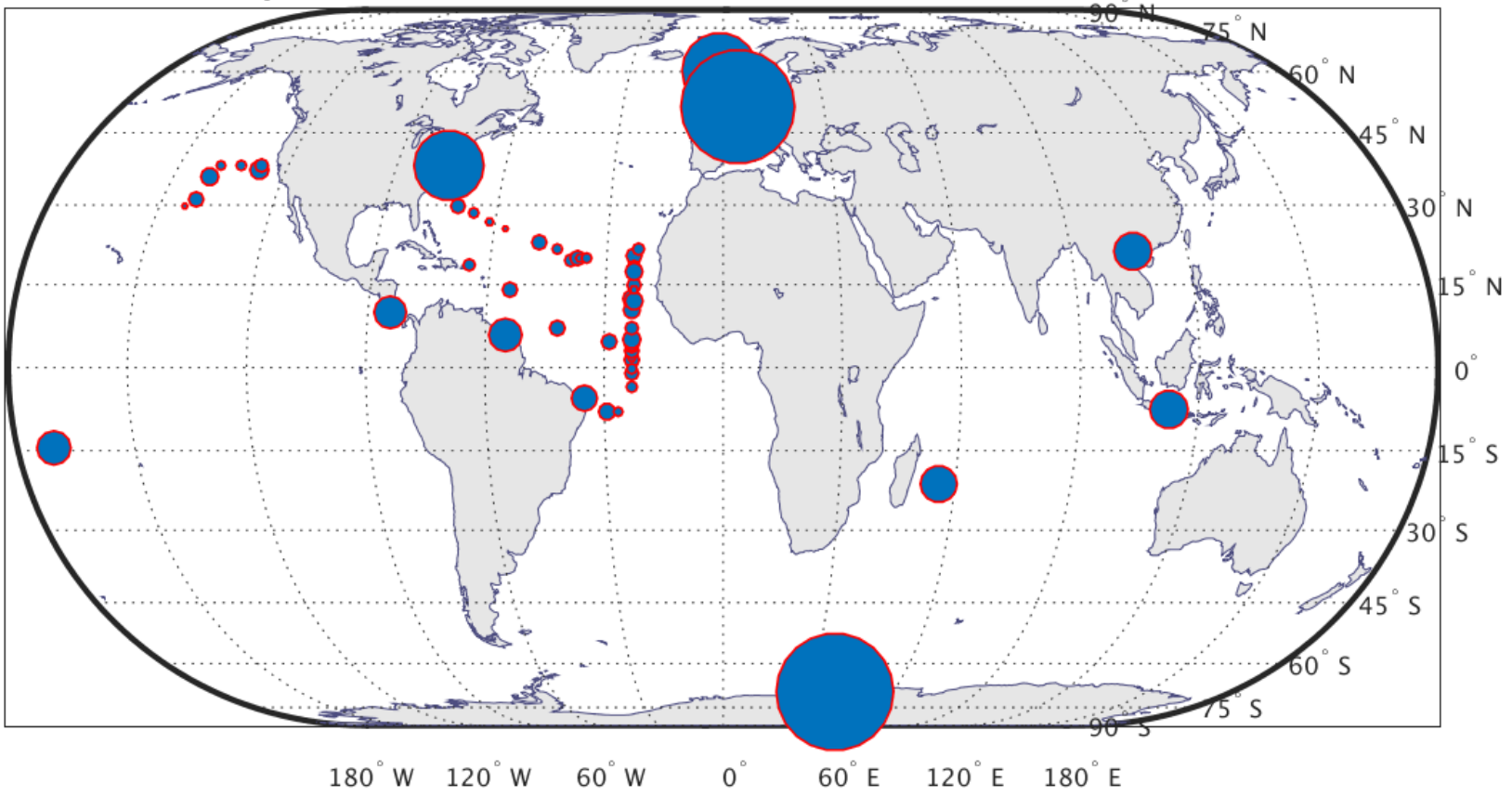
IR Ozone Profile EDR Validation (2/8)

VALAR Ozonesonde-FOR Collocation Sample (*n* = 6024)

Geographic Histogram (Equal Area)

FOR Collocation Criteria: $\delta x \leq 125$ km, $-240 < \delta t < +120$ min

valar_nucaps_offline_v15_collocation_file_o3_shadoz-raob_20160805.mat

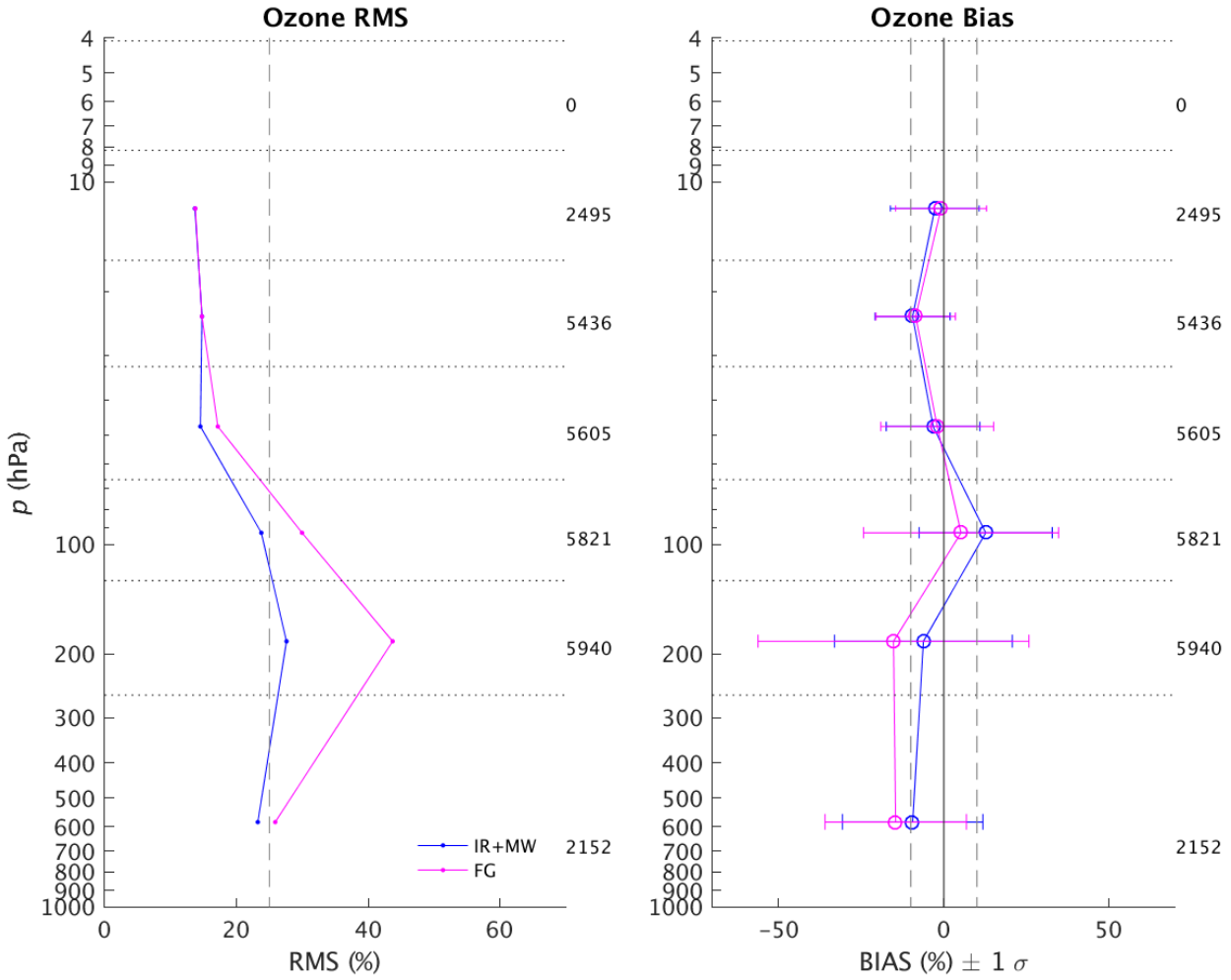


IR Ozone Profile EDR Validation (3/8)

NUCAPS Offline (v1.5) versus Global Ozonesondes

Retrieval and ***A Priori*** **First Guess**

IR+MW Yield = 62.2%

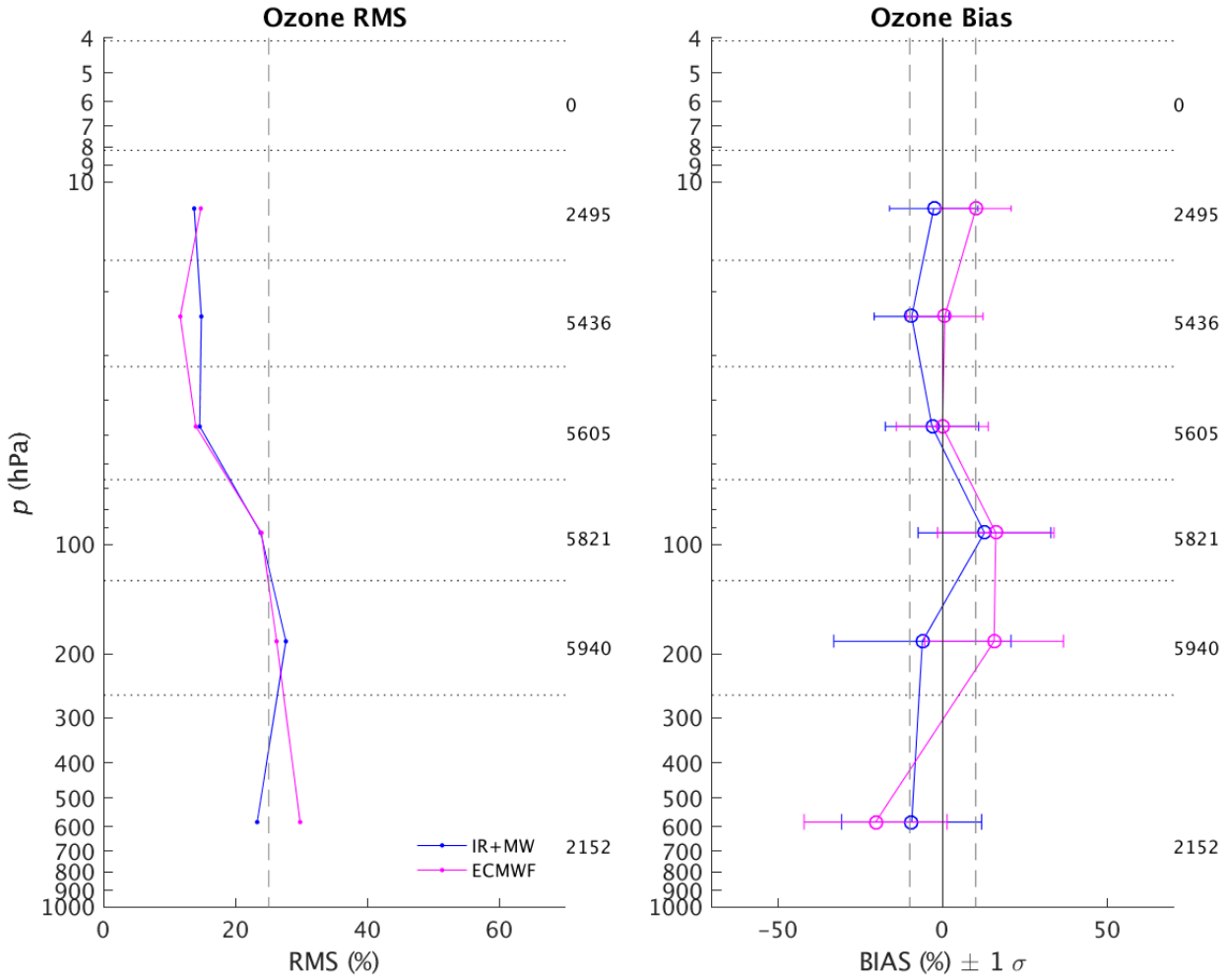


IR Ozone Profile EDR Validation (4/8)

NUCAPS Offline (v1.5) versus Global Ozonesondes

Retrieval and **ECMWF**

IR+MW Yield = 62.2%



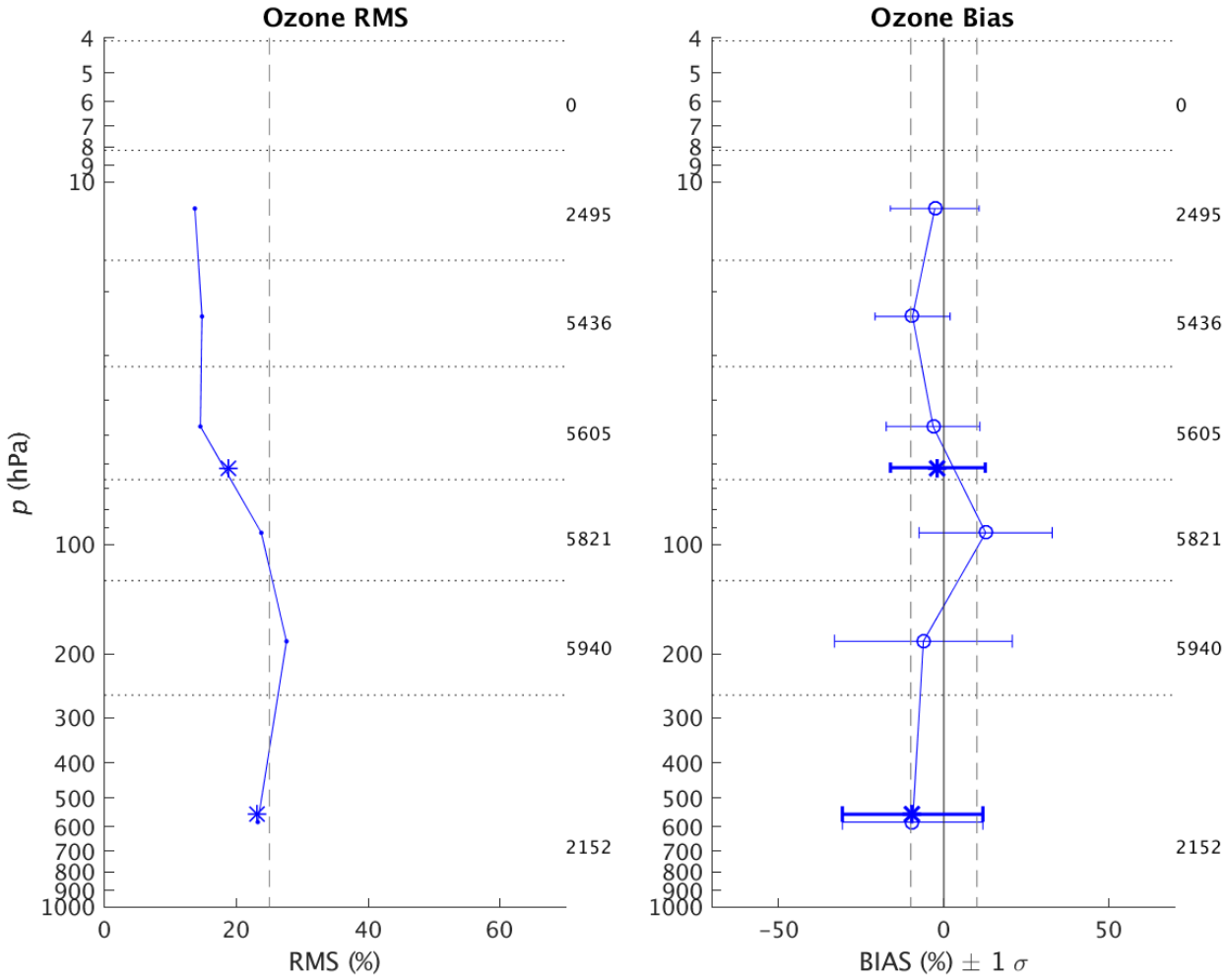
IR Ozone Profile EDR Validation (5/8)

NUCAPS Offline (v1.5) versus Global Ozonesondes

* Broad-Layer Statistics

(Per JPSS Level 1 Requirements)

IR+MW Yield = 62.2%



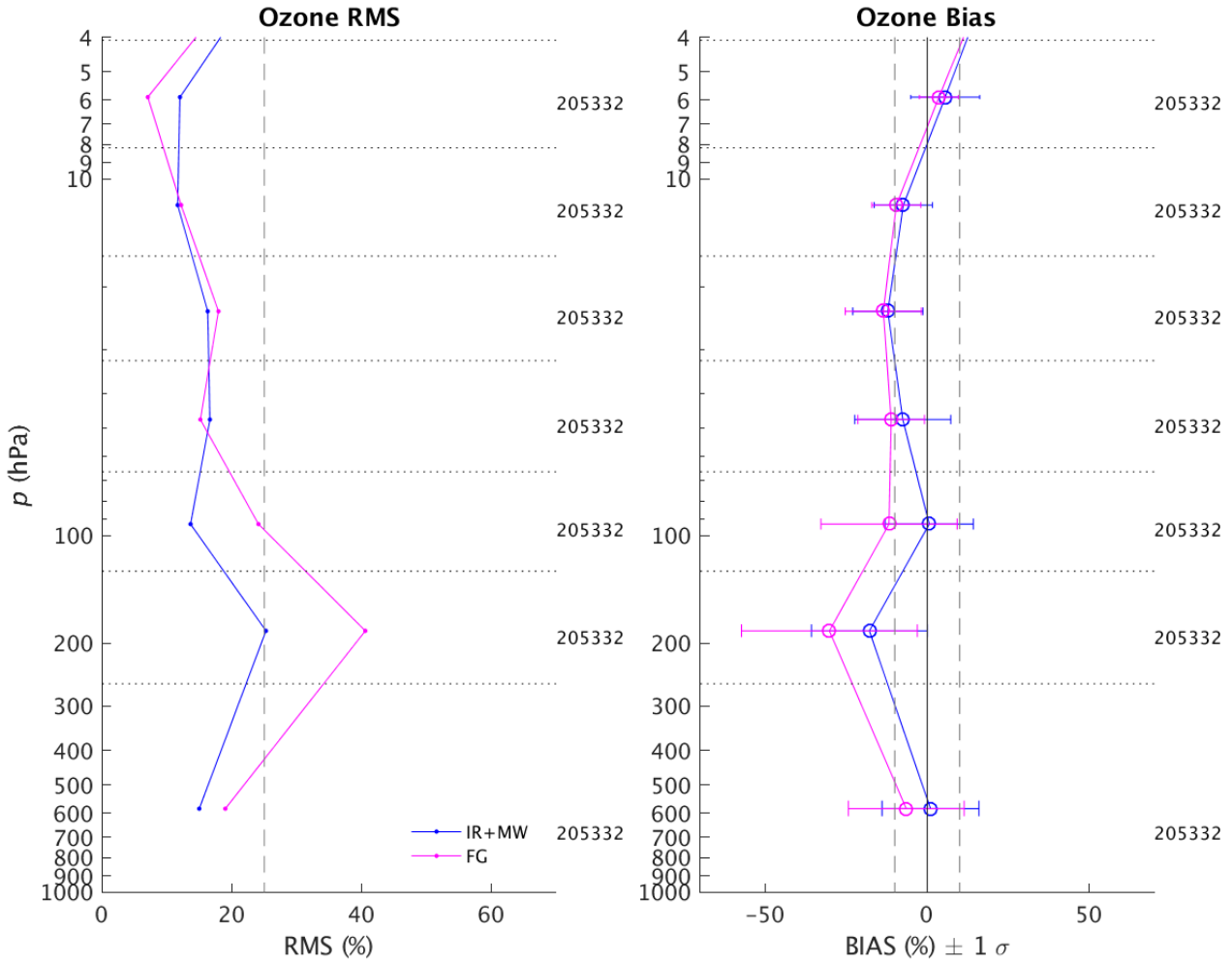
IR Ozone Profile EDR Validation (6/8)

NUCAPS Offline (v1.5) versus Global Focus Day 17-Feb-2015

O_3 Versus ECMWF

IR+MW
First Guess

NUCAPS v1.5
Yield = 63.4%



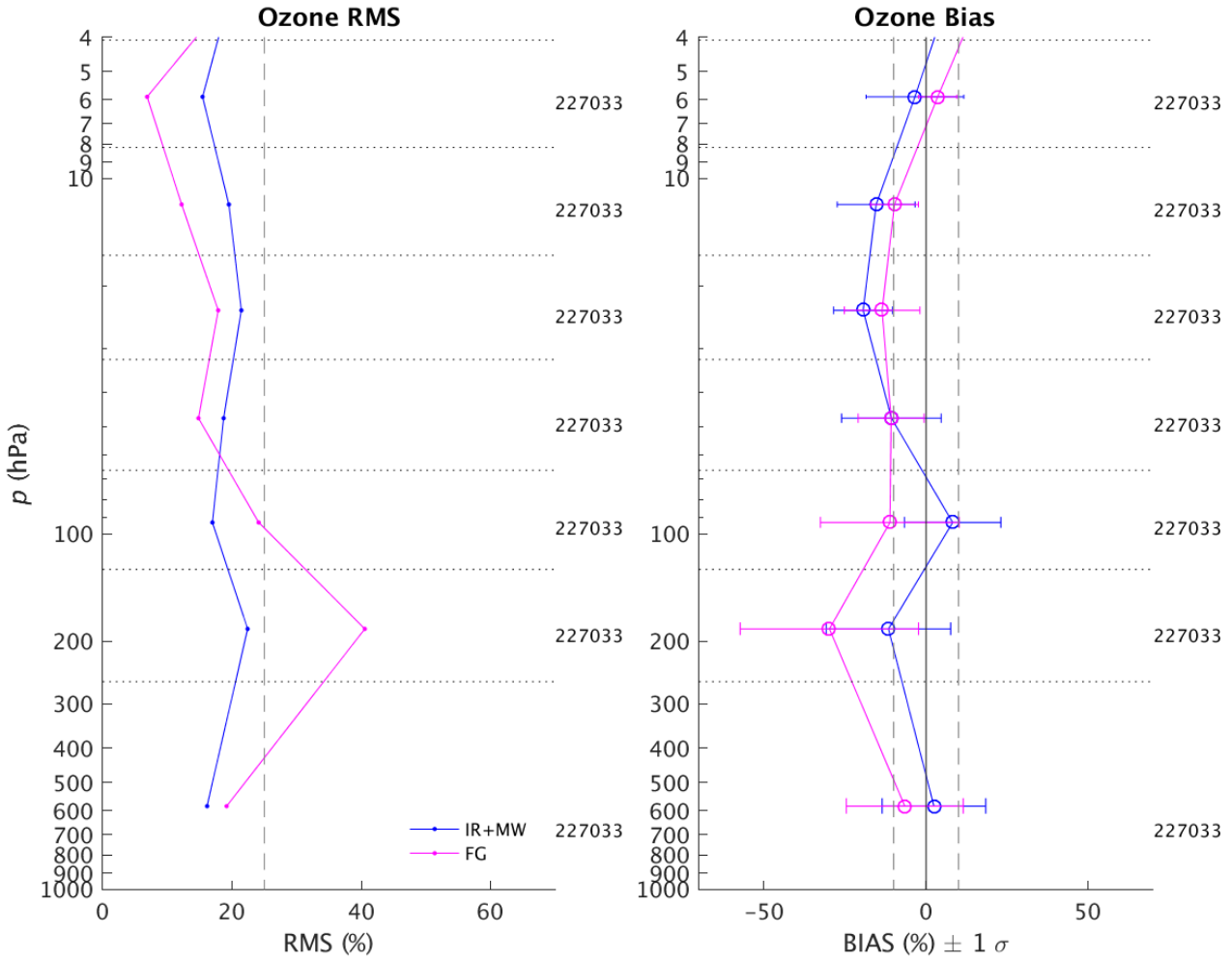
IR Ozone Profile EDR Validation (7/8)

NUCAPS Offline (v1.8.1) versus Global Focus Day 17-Feb-2015

O_3 Versus ECMWF

IR+MW
First Guess

NUCAPS v1.8.1
Yield = 70.1%



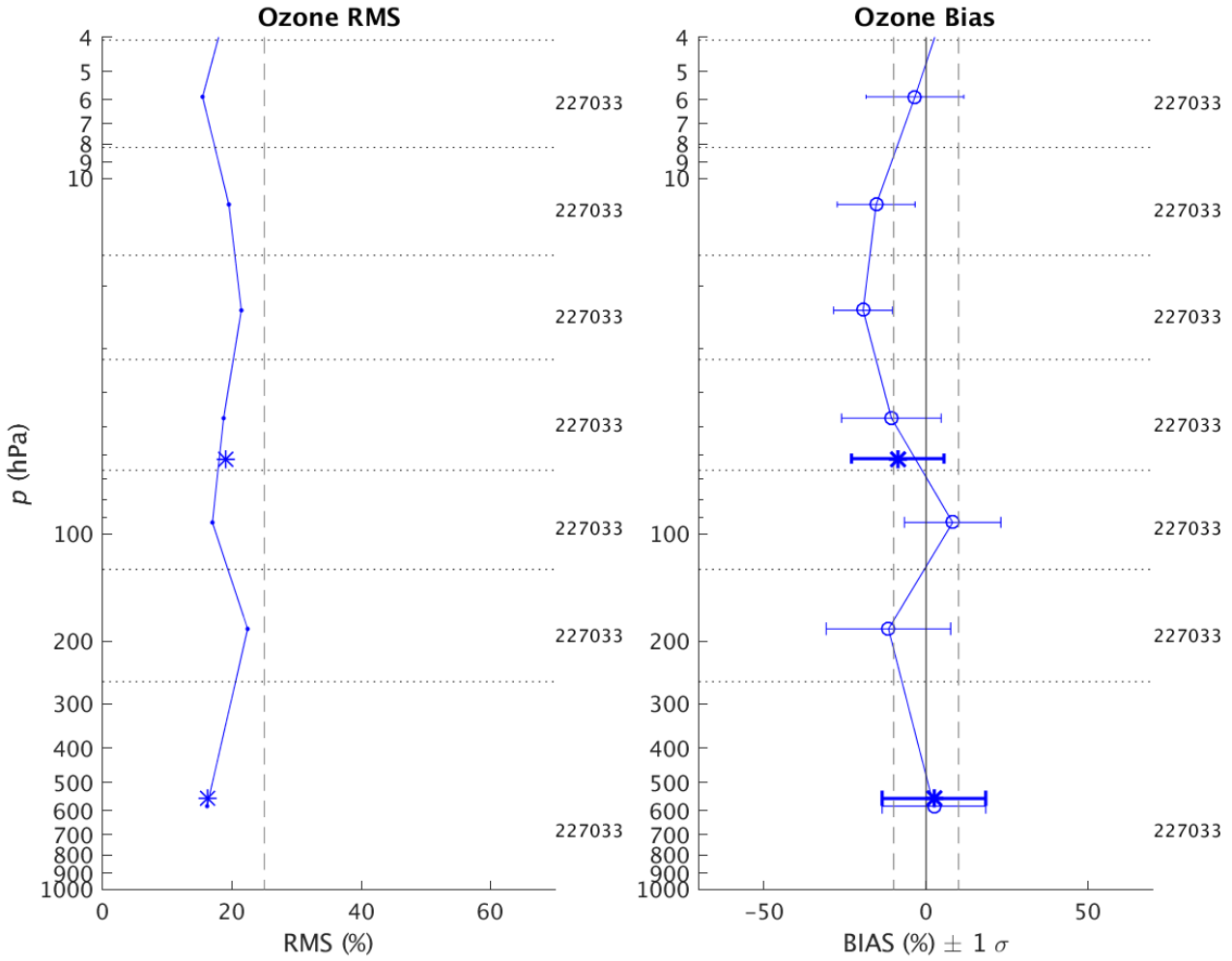
IR Ozone Profile EDR Validation (8/8)

NUCAPS Offline (v1.8.1) versus Global Focus Day 17-Feb-2015

* Broad-Layer Statistics

(Per JPSS Level 1 Requirements)

NUCAPS v1.8.1
Yield = 70.1%



Validation of SNPP NUCAPS trace gas EDRs

CARBON MONOXIDE (PRELIMINARY)

Basic Methodology for CO and CO_2

- The **AIRS v6 standard products** were obtained for the global Focus day 17 February 2015
  - Total column integrated CO and CH_4
  - The AIRS Team provided us offline runs for CO_2
- AIRS and NUCAPS were divided into ascending (ASC) and descending (DES) orbits
- Linear interpolations of FOR (lat/lon) were then performed for each orbit (ASC and DES) to create a one-to-one correspondence of collocation data points
  - AIRS CO was interpolated to NUCAPS
  - NUCAPS CO_2 was interpolated to the more sparse AIRS

- **NUCAPS offline runs for** global **Focus Day 17 February 2015**
  - **v1.5 (nominal CrIS res)**
  - **v1.8.1 (full CrIS res)**

- **For NUCAPS CO,** profile EDRs on 100 RTA layers are integrated to obtain total column abundances (molecules/cm2) according to *Nalli et al.* (2013)

$$\Sigma_x(z) \equiv \int_{z_t}^{z} N_x(z')\,\mathrm{d}z'$$

$$\Longrightarrow \quad \Sigma_x(z) \approx \Sigma_{x,\mathcal{L}} \equiv \sum_{\mathcal{L}}^{n_{\mathcal{L}}} \overline{N}_{x,\mathcal{L}}\ \delta z_{\mathcal{L}}$$

with stats being computed relative to the AIRS v6 total column product

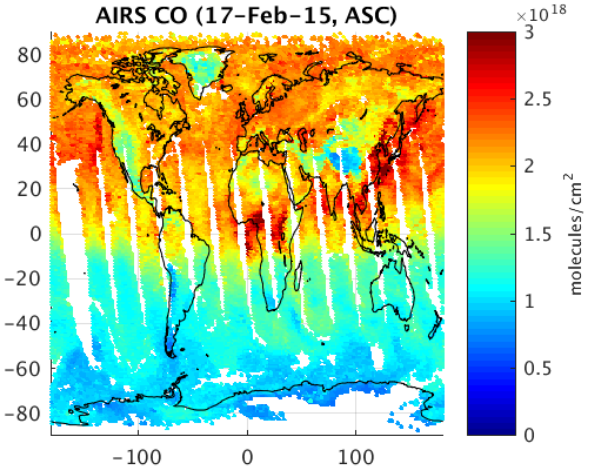
- **For NUCAPS CO_2,** stats are performed simply for atmospheric column averages (in PPMV)

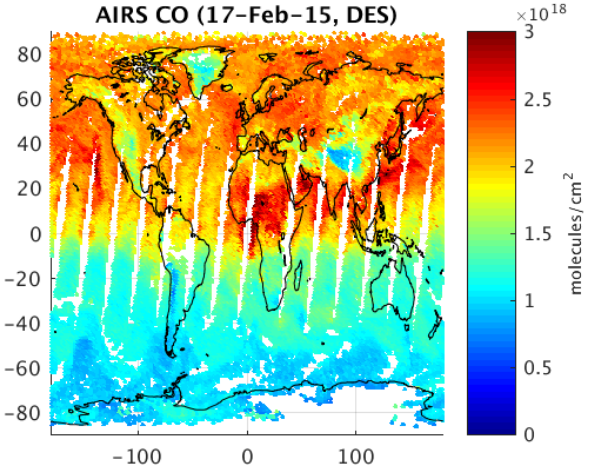
Total Column Carbon Monoxide (CO) EDR (1/2)

17 Feb 2015 Focus Day, NUCAPS v1.5 and AIRS v6 Accepted Cases

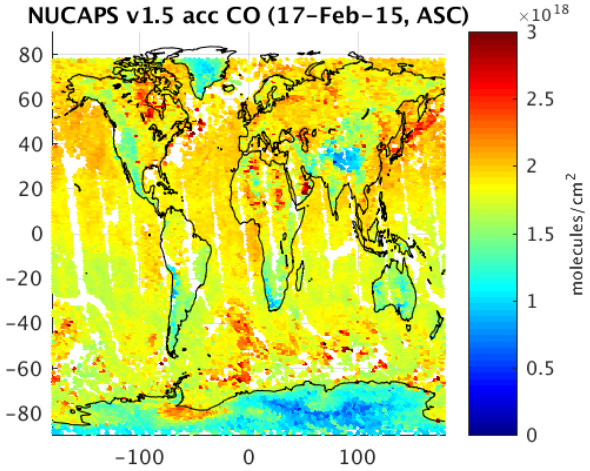
Preliminary

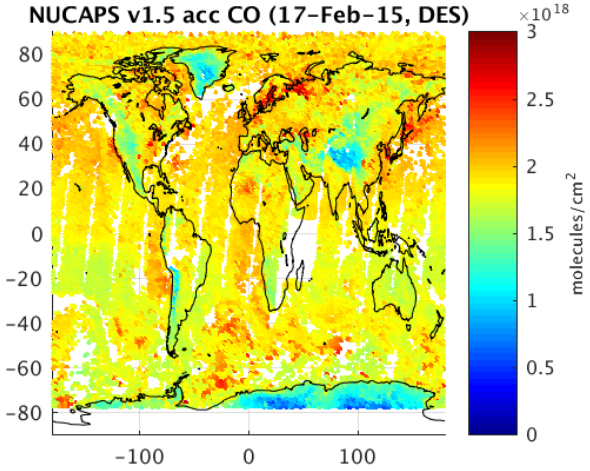
AIRS v6





NUCAPS v1.5





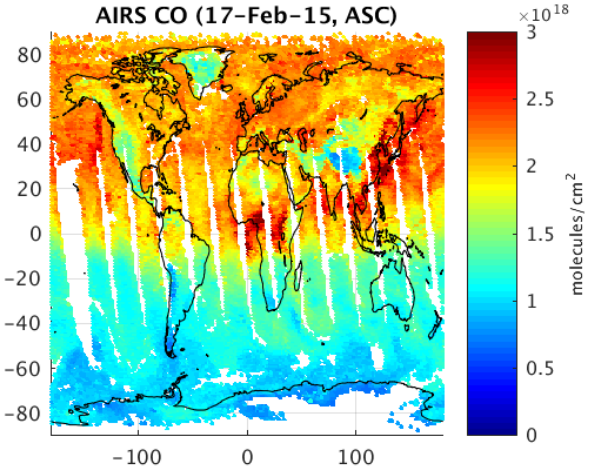
NUCAPS v1.5
Yield = 63.4%

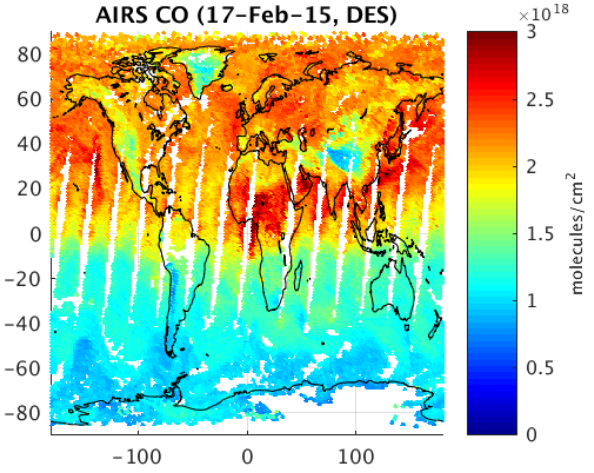
Total Column Carbon Monoxide (CO) EDR (2/2)

17 Feb 2015 Focus Day, NUCAPS v1.8.1 and AIRS v6 Accepted Cases

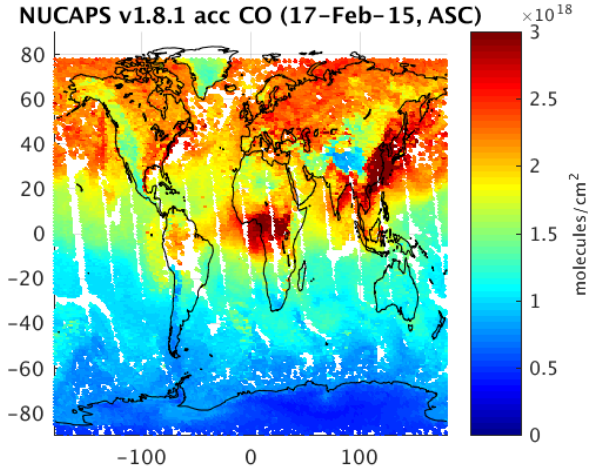
Preliminary

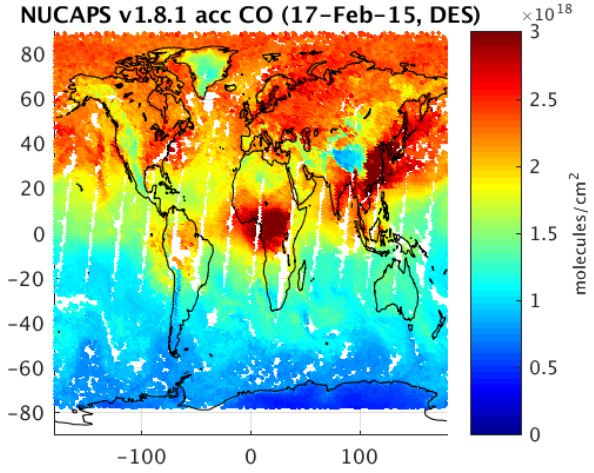
AIRS v6





NUCAPS v1.8.1





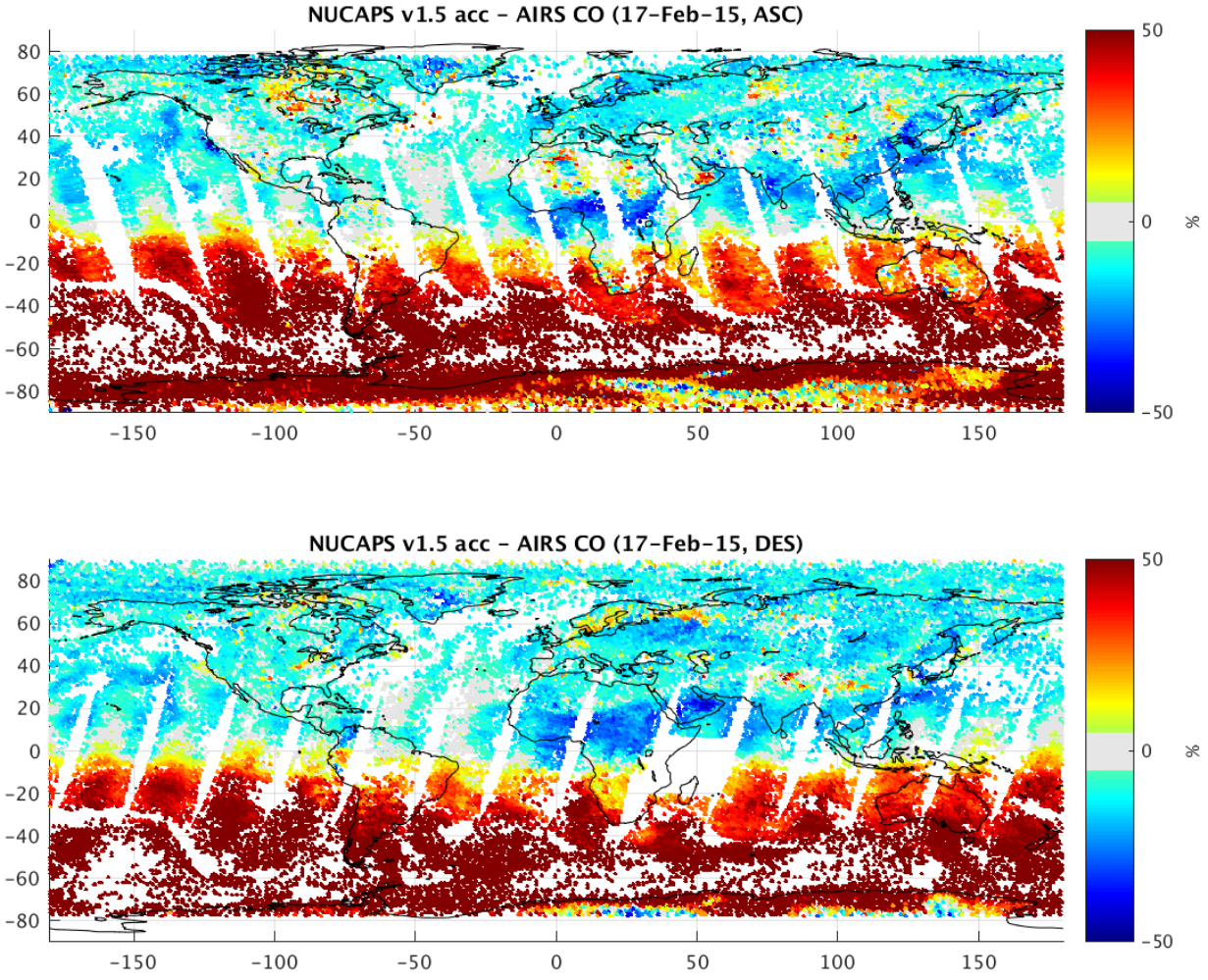
NUCAPS v1.8.1
Yield = 70.1%

NUCAPS v1.5 CO – AIRS v6 CO

17 Feb 2015 Focus Day, Accepted Cases

Preliminary

NUCAPS v1.5 (Nominal CrIS Resolution)

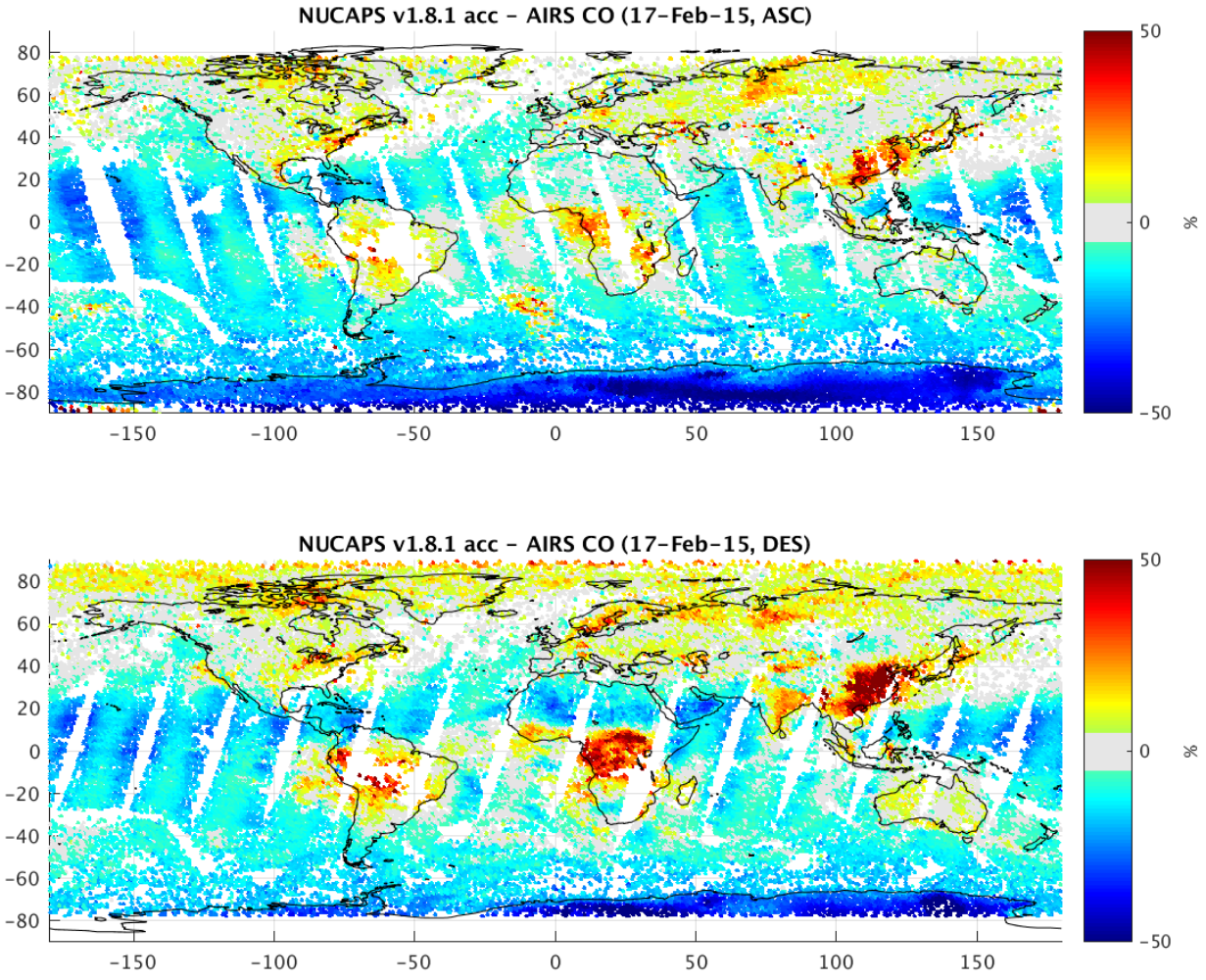


NUCAPS v1.8.1 CO – AIRS v6 CO

17 Feb 2015 Focus Day, Accepted Cases

Preliminary

NUCAPS v1.8.1 (Full CrIS Resolution)



Validation of SNPP NUCAPS trace gas EDRs

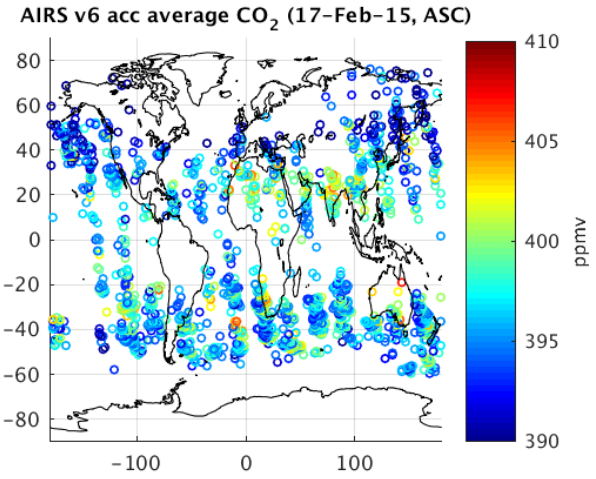
CARBON DIOXIDE (PRELIMINARY)

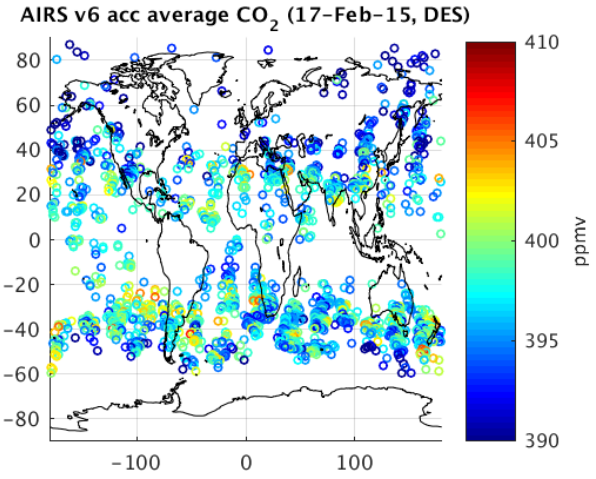
Mean Column Carbon Dioxide (CO_2) EDR (1/2)

17 Feb 2015 Focus Day, NUCAPS v1.5 and AIRS v6 Accepted Cases

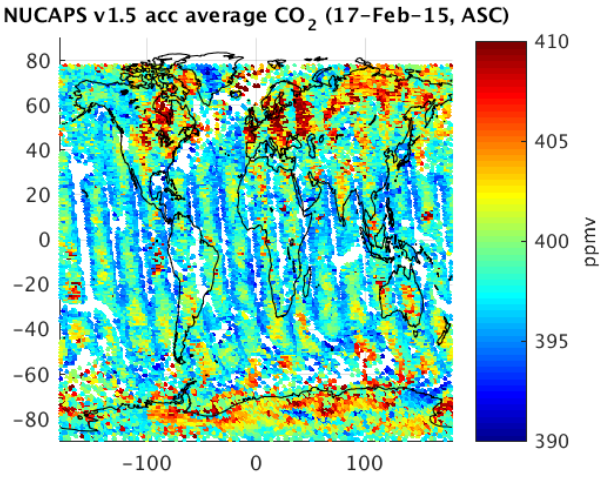
Preliminary

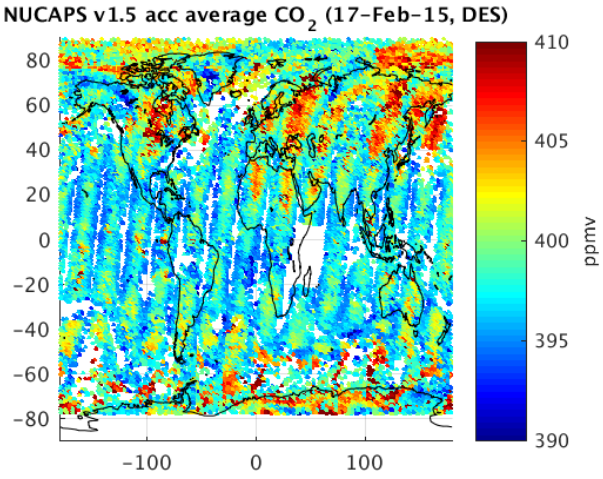
AIRS v6





NUCAPS v1.5





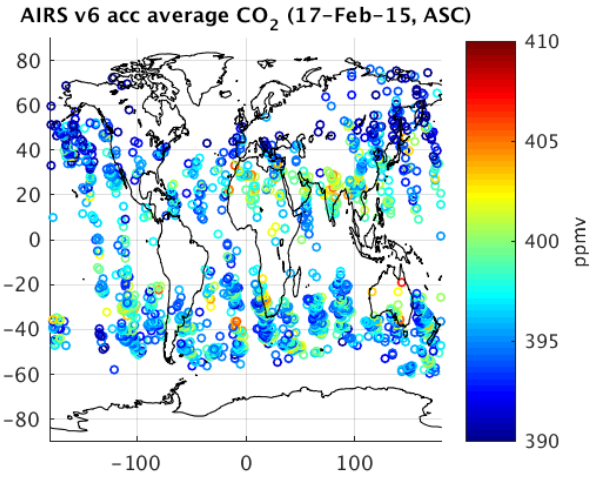
NUCAPS v1.5
Yield = 63.4%

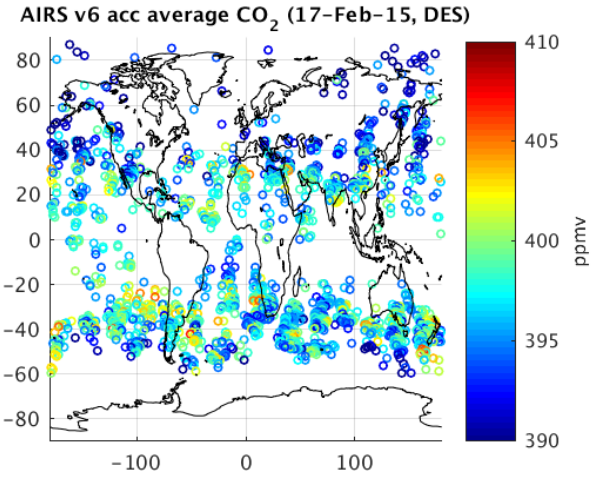
Mean Column Carbon Dioxide (CO_2) EDR (1/2)

17 Feb 2015 Focus Day, NUCAPS v1.8.1 and AIRS v6 Accepted Cases

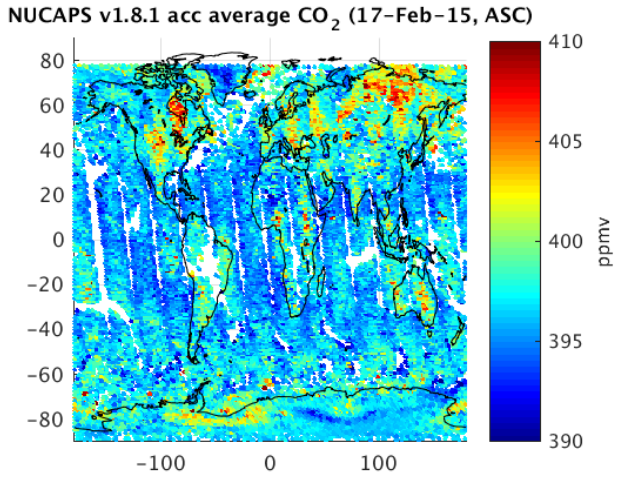
Preliminary

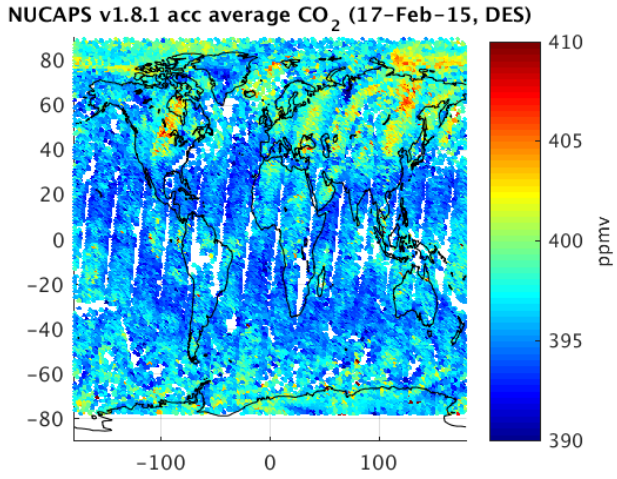
AIRS v6





NUCAPS v1.8.1





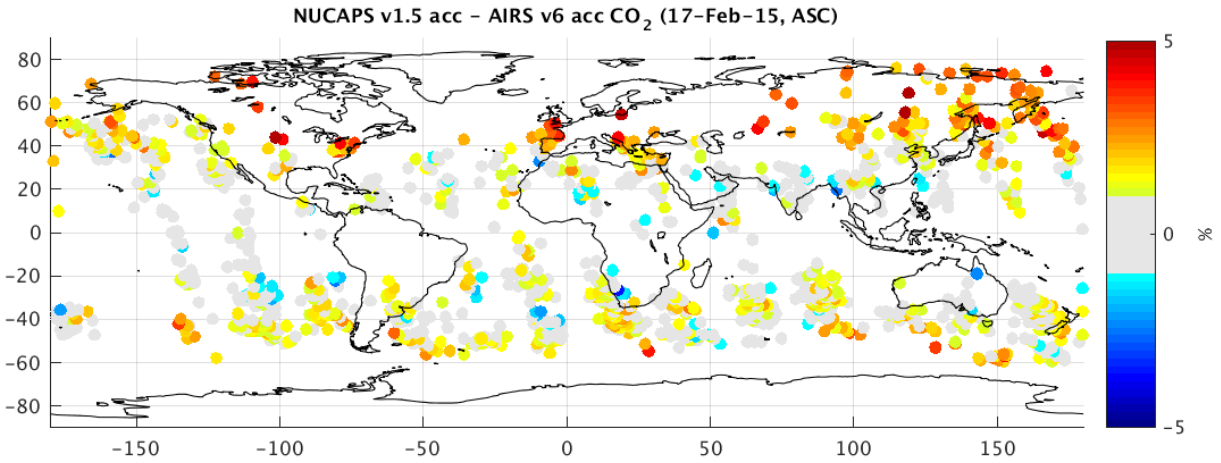
NUCAPS v1.8.1
Yield = 70.1%

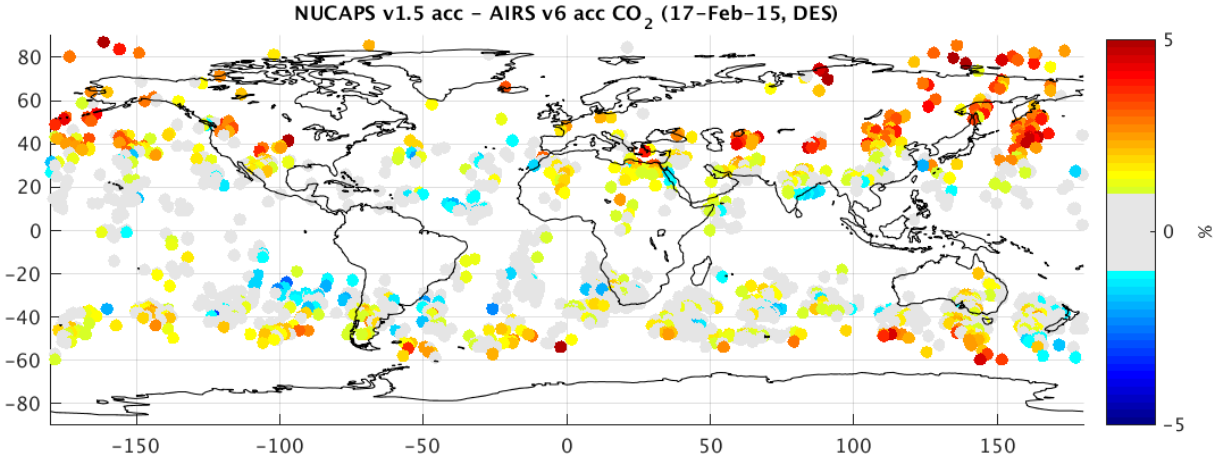
NUCAPS v1.5 CO_2 – AIRS v6 CO_2

17 Feb 2015 Focus Day, NUCAPS and AIRS Accepted Cases

Preliminary

NUCAPS v1.5 (Nominal CrIS Resolution)



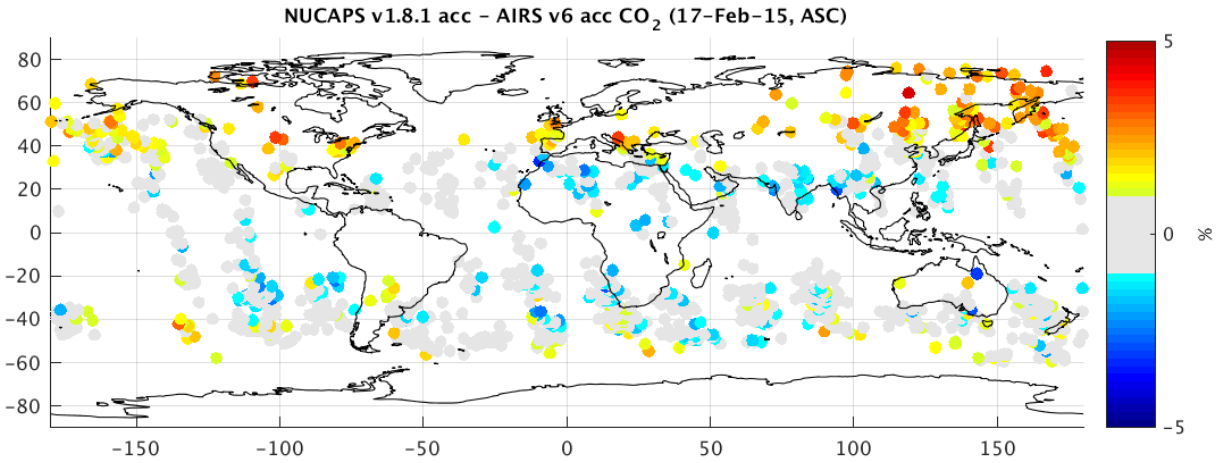


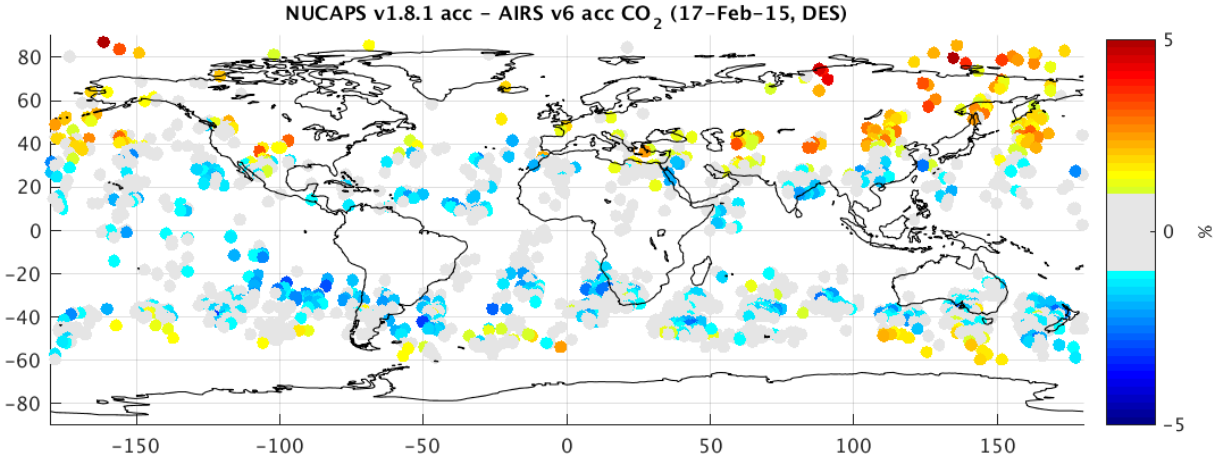
NUCAPS v1.8.1 CO_2 – AIRS v6 CO_2

17 Feb 2015 Focus Day, NUCAPS and AIRS Accepted Cases

Preliminary

NUCAPS v1.8.1 (Full CrIS Resolution)





Preliminary Global Statistics NUCAPS versus AIRS
(accepted cases)

	V1.5 CrIS Nom Res			V1.8.1 CrIS Full Res		
Trace Gas EDR	**BIAS (%)**	**STD (%)**	**RMS (%)**	**BIAS (%)**	**STD (%)**	**RMS (%)**
CO (asc)	**+21.7** (±25.0)	**41.5** (35.0)	46.8	**−10.3** (±5.0)	**28.1** (15.0)	17.8
CO (des)	**+11.0** (±25.0)	**33.4** (35.0)	35.1	**−3.2** (±5.0)	**14.8** (15.0)	15.7
CO_2 (asc)	**+0.9** (±1.0)	**1.1** (0.5)	1.4	**+0.2** (±1.0)	**1.1** (0.5)	1.4
CO_2 (des)	**+0.8** (±1.0)	**1.2** (0.5)	1.5	**−0.2** (±1.0)	**1.2** (0.5)	1.4

O_3, CO, CO_2 Trace Gas Summary

- The **NUCAPS IR ozone (O_3) profile EDR products are shown to meet JPSS Level 1 requirements**
  - The **offline v1.5 (nominal CrIS resolution) ozone EDR** has reached **"Validated Maturity"** based upon coarse/broad layer statistical analyses versus
    - Collocated **global ozonesondes**, including **dedicated ozonesondes** (Validation Hierarchy Method #4)
    - **Global Focus Day** (17 February 2015) **ECMWF** output (Validation Hierarchy Method #1)
  - The **offline v1.8.1 (full CrIS resolution) also meets Level 1 requirements** based upon coarse/broad layer statistical analyses versus
    - **Global Focus Day ECMWF** output
    - **Statistics are comparable to the ozonesonde-validated NUCAPS v1.5**

- For validation of **NUCAPS carbon monoxide (CO)** and **carbon dioxide (CO_2) EDRs**, we rely on satellite EDR Intercomparisons (Validation Hierarchy Method #2) versus **collocated AIRS v6**
  - **AIRS flown on Aqua is in the same orbit as SNPP** and is thus ideal for collocations with SNPP
  - **NUCAPS v1.5 CO** and **CO_2** retrievals **meet the relaxed JPSS Level 1 requirements for BIAS**
  - **NUCAPS v1.5 and v1.8.1 CO descending orbit currently meet JPSS Level 1 requirements**

- **Future Work**
  - **Perform "spot-checks" of AIRS and NUCAPS EDRs using *in situ* datasets of opportunity**
  - Utilize a larger data sample (e.g., month) for the CO_2 validation, apply other techniques for QA (e.g., considering DOF, applying AKs, etc.)
  - Further optimization of NUCAPS full-resolution algorithm
  - Investigate improvements in the ozone *a priori*

SNPP NUCAPS Validation

THANK YOU! QUESTIONS?